

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090319\
 Data File : BM022512.D
 Acq On : 03 Sep 2019 20:47
 Operator : HP/JU
 Sample : K4563-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CIW-6S-(0-4)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.128	358	364	377	rBV	382596	576826	43.82%	8.100%
2	6.704	626	632	647	rBV	370633	624199	47.42%	8.765%
3	7.039	683	689	700	rBV	465789	694566	52.77%	9.753%
4	7.504	762	768	775	rBB	86030	132213	10.04%	1.857%
5	7.810	814	820	831	rBB	351366	537900	40.87%	7.553%
6	8.681	961	968	982	rBV	185904	372998	28.34%	5.238%
7	10.280	1234	1240	1257	rBV	71496	144465	10.98%	2.029%
8	12.769	1657	1663	1676	rBV	541018	814389	61.87%	11.436%
9	13.533	1786	1793	1798	rBV2	19257	28927	2.20%	0.406%
10	13.610	1802	1806	1809	rVV2	14513	20446	1.55%	0.287%
11	13.657	1809	1814	1821	rVB	23934	43329	3.29%	0.608%
12	13.957	1860	1865	1871	rVB5	14230	25198	1.91%	0.354%
13	14.168	1896	1901	1909	rBV	117992	183434	13.94%	2.576%
14	14.663	1980	1985	1992	rBV5	8924	16832	1.28%	0.236%
15	14.786	1997	2006	2012	rBV5	6921	18157	1.38%	0.255%
16	14.921	2025	2029	2035	rBV3	11020	15257	1.16%	0.214%
17	15.680	2152	2158	2175	rBV	478540	773739	58.78%	10.865%
18	15.886	2187	2193	2197	rBV3	8121	16406	1.25%	0.230%
19	16.939	2367	2372	2384	rBV2	119054	210502	15.99%	2.956%
20	17.827	2519	2523	2531	rBV5	22161	35684	2.71%	0.501%
21	19.127	2739	2744	2748	rBV2	9556	14765	1.12%	0.207%
22	19.580	2815	2821	2831	rBV	1051037	1316234	100.00%	18.483%
23	20.844	3032	3036	3042	rBV3	32518	50718	3.85%	0.712%
24	21.162	3085	3090	3107	rBV	147497	238239	18.10%	3.345%
25	23.344	3456	3461	3474	rVB2	97035	215972	16.41%	3.033%

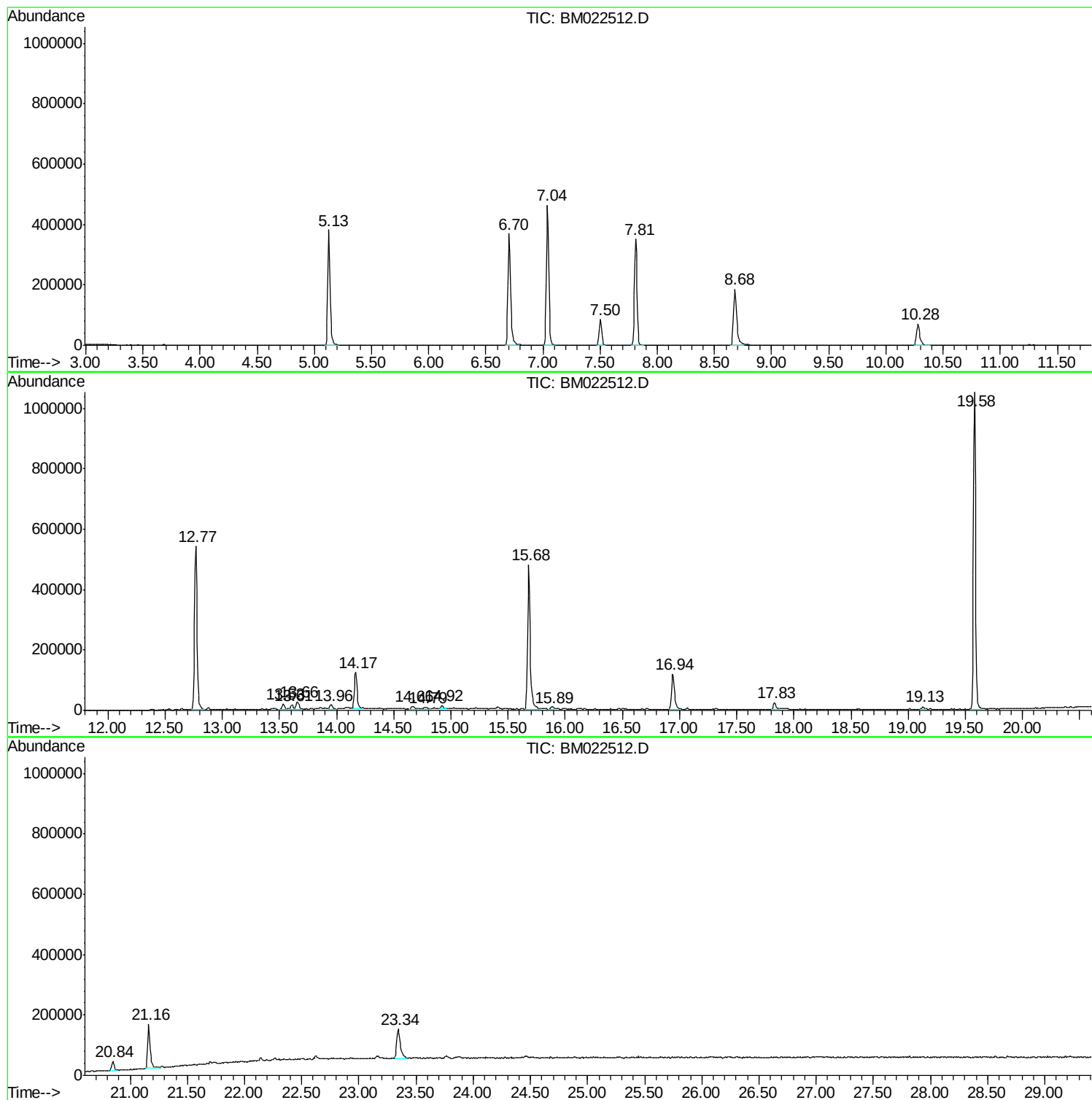
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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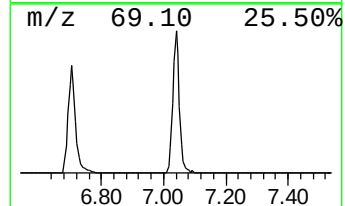
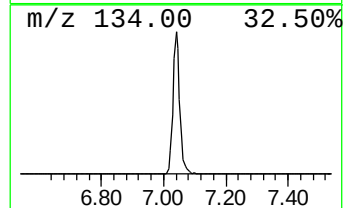
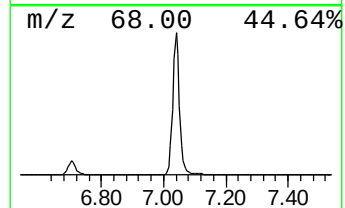
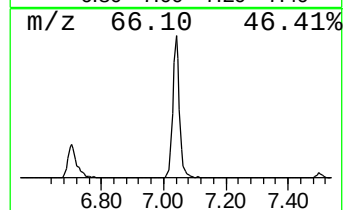
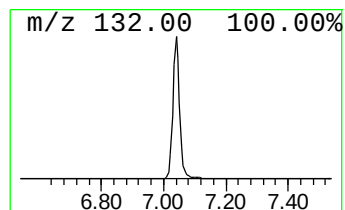
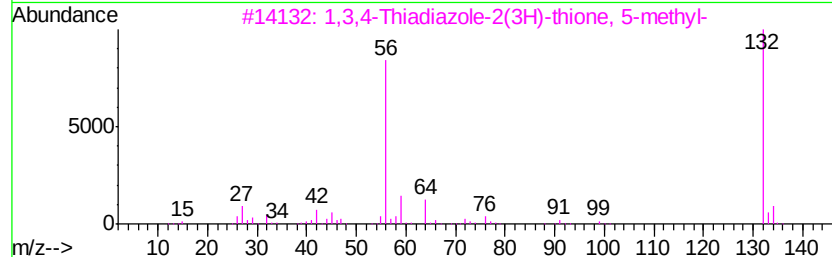
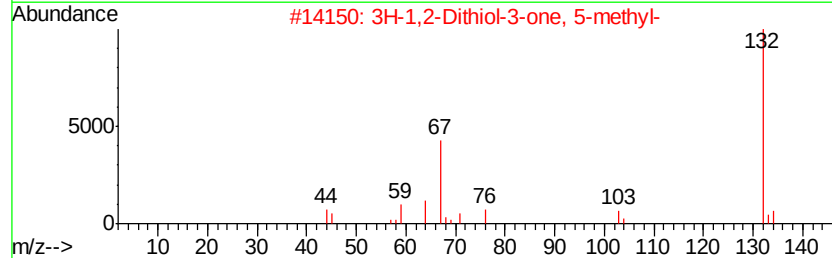
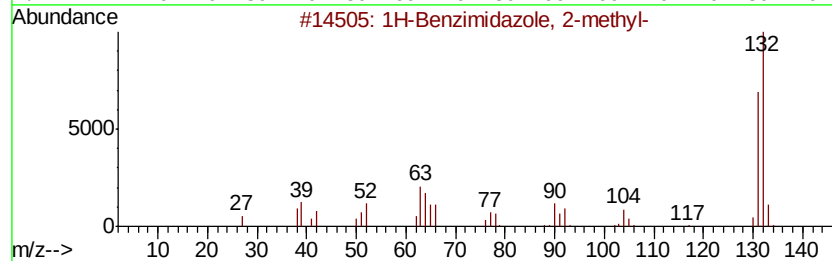
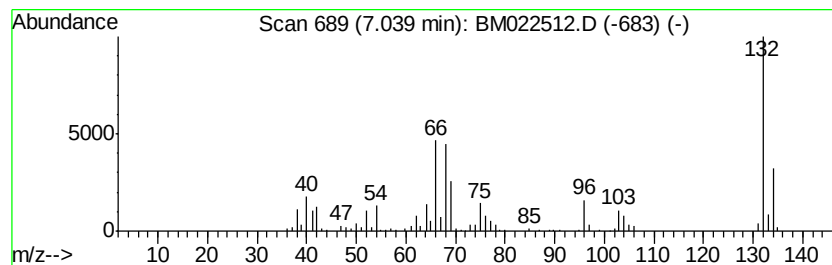
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	105.07 ng	694566	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	18
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	14
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10



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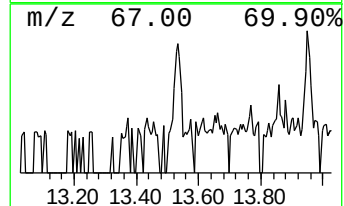
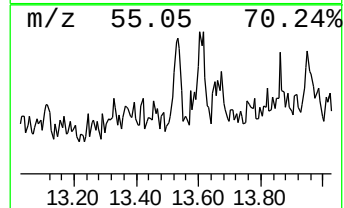
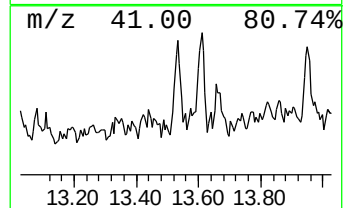
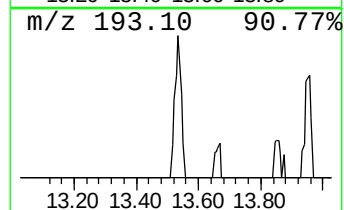
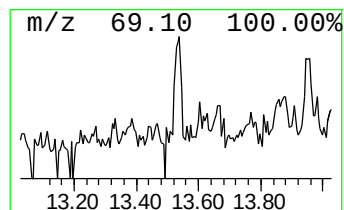
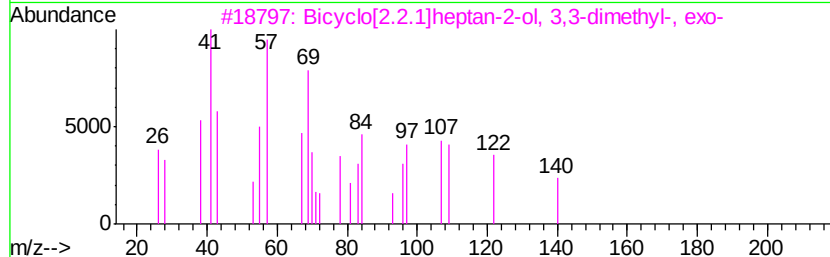
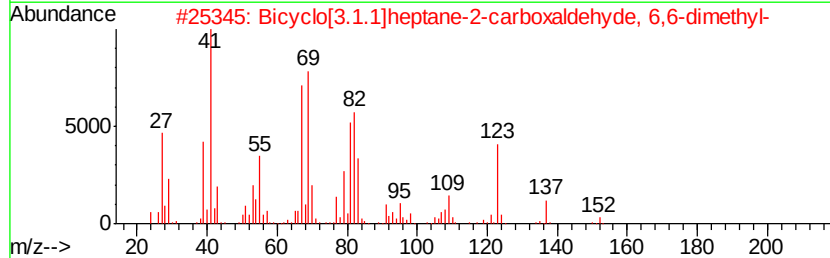
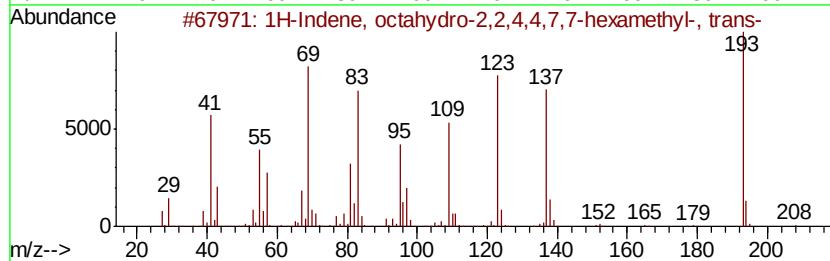
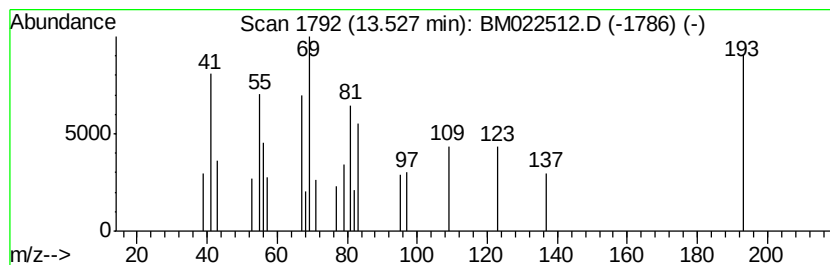
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Peak Number 3 unknown13.53 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	3.15 ng	28927	Acenaphthene-d10	14.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
2		Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	35
3		Bicyclo[2.2.1]heptan-2-ol, 3,3-d...	140	C9H16O	000515-28-6	32
4		Disparlure	282	C19H38O	029804-22-6	30
5		1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-25-7	27



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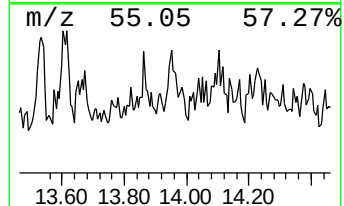
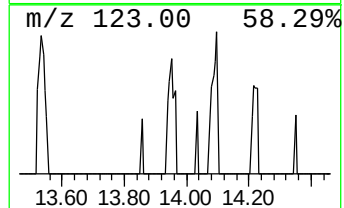
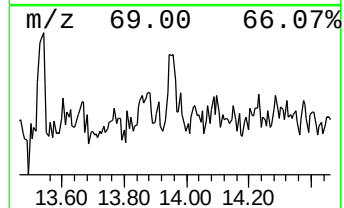
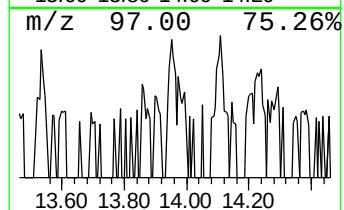
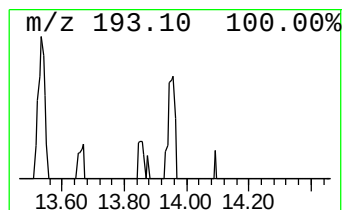
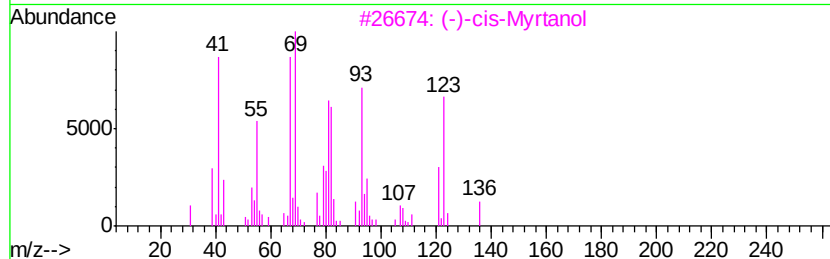
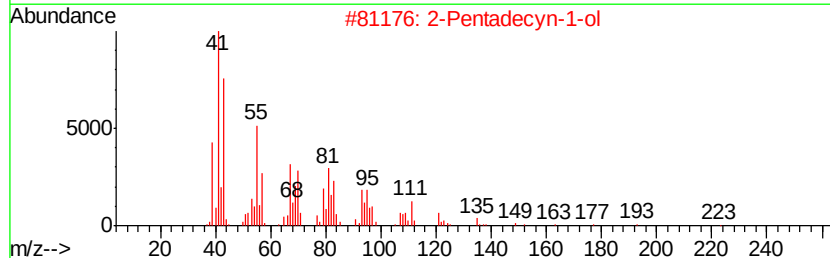
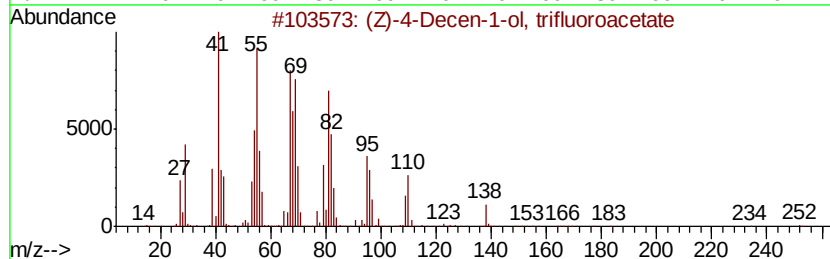
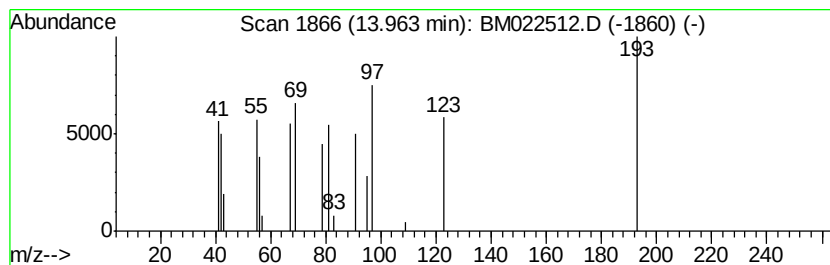
Instrument :
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Peak Number 4 unknown13.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.96	2.75 ng	25198	Acenaphthene-d10	14.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-4-Decen-1-ol, trifluoroacetate	252	C12H19F3O2	1000352-33-5	14
2	2-Pentadecyn-1-ol	224	C15H28O	002834-00-6	12
3	(-)-cis-Mvrtanol	154	C10H18O	051152-12-6	10
4	2-Octylcyclopropene-1-heptanol	266	C18H34O	054467-85-5	10
5	Undecane, 1,2-dibromo-2-methyl-	326	C12H24Br2	055334-43-5	10



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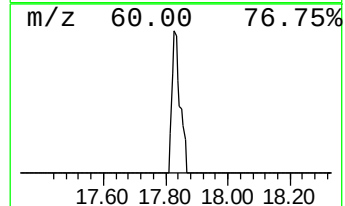
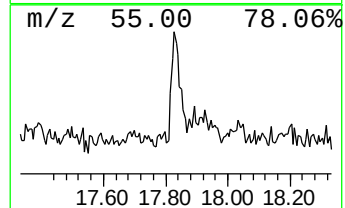
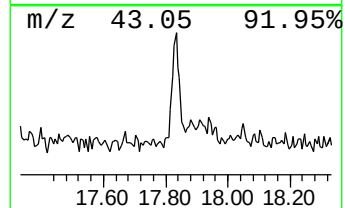
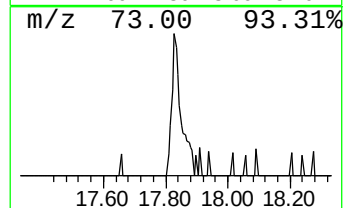
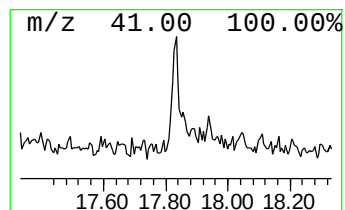
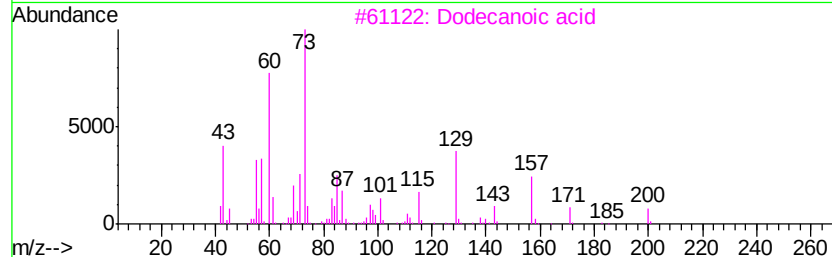
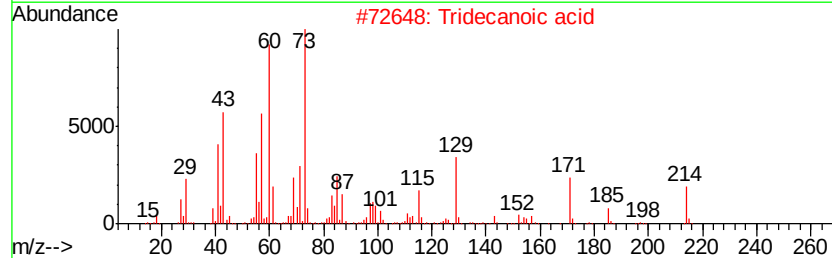
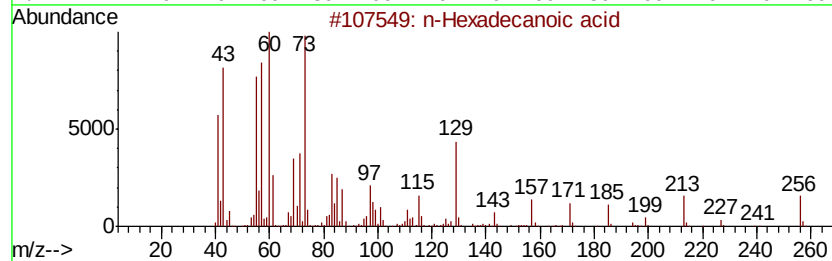
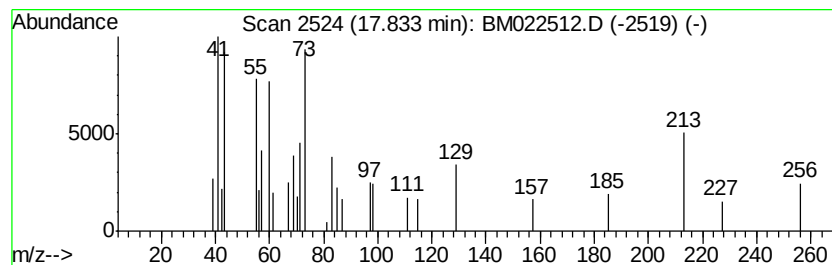
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	3.39 ng	35684	Phenanthrene-d10	16.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
2		Tridecanoic acid	214	C13H26O2	000638-53-9	47
3		Dodecanoic acid	200	C12H24O2	000143-07-7	46
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	38



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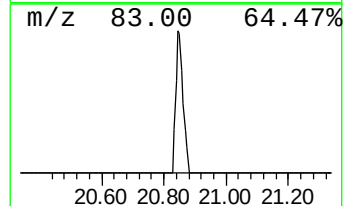
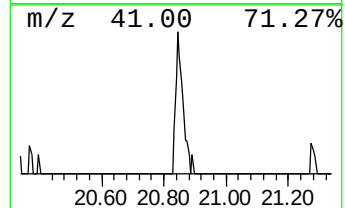
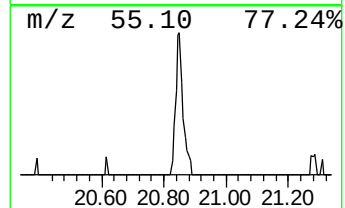
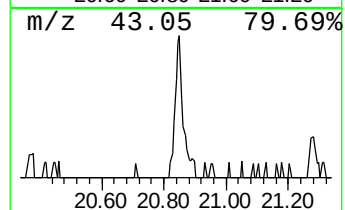
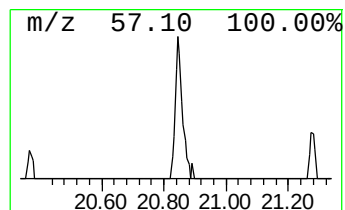
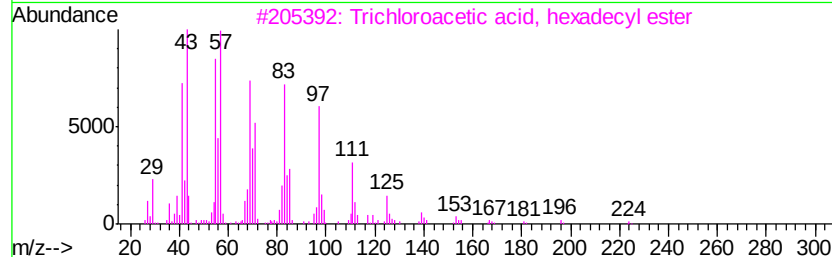
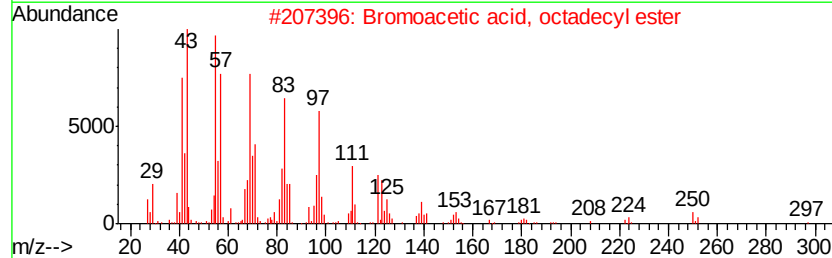
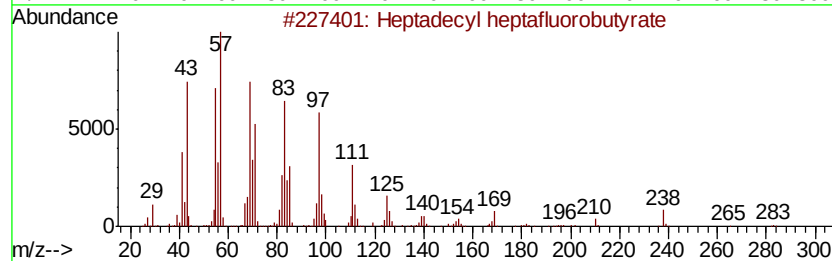
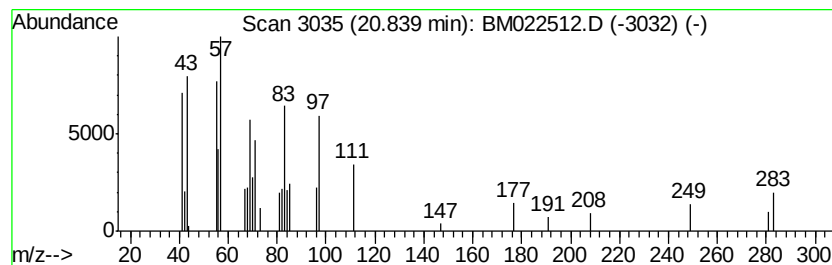
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Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	4.26 ng	50718	Chrysene-d12	21.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.04	7.04	105.1	ng	694566	1	7.50	132213	20.0
unknown13.53	13.53	3.1	ng	28927	3	14.17	183434	20.0
unknown13.96	13.96	2.8	ng	25198	3	14.17	183434	20.0
n-Hexadecanoic acid	17.83	3.4	ng	35684	4	16.94	210502	20.0
Heptadecyl heptaf...	20.84	4.3	ng	50718	5	21.16	238239	20.0